COMPUTER VISION FOR UNDERSTANDING INDUSTRIAL REACTION KINETICS ACROSS SCALES

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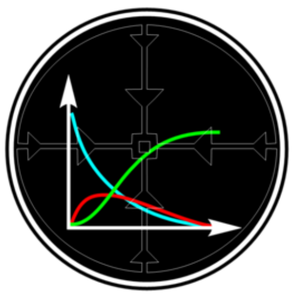
Introduction

Computer vision combines camera and software to analyse real world phenomena.

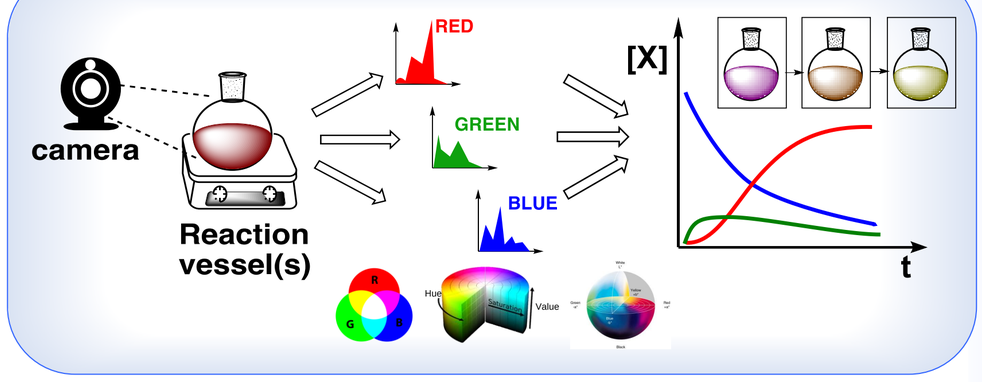
It is already widely applied across a range of sectors,[1] including the automotive, aerospace, and food processing industries.[2]

We record chemical processes on the small and large scale using carefully selected cameras without ever touching the vessel.



Kineticolor

Video analysis for colour kinetics at any scale.



All computer vision-enabled colour analysis is achieved using the *Kineticolor* program that is being developed within Reid Group Research at the University of Strathclyde.

Pd catalysis

Metal catalyst degradation presents challenges in cost, efficiency, purification, safety, and waste profile of reactions scales of synthesis.[3]

Tracking Pd Catalyst Degradation

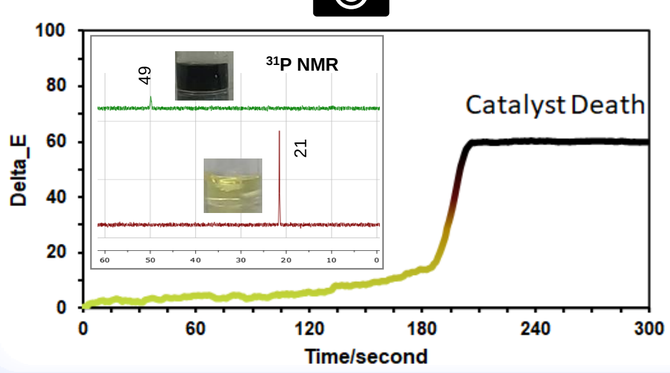
Pre-catalyst
$[(Cy_3P)_2Pd(OAc)_2]$

B_2Pin_2 (10 equiv.)
Exposed to Air

Toluene, 70 °C, 5 min

Camera Monitoring

Pd black



Pre-catalyst
Air-stable
$[(R_3P)_2Pd^{II}X_2]$

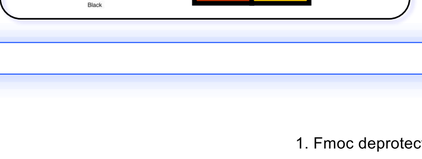
activation

Active Catalyst
Air-sensitive
$[(R_3P)_2Pd^{0}]$

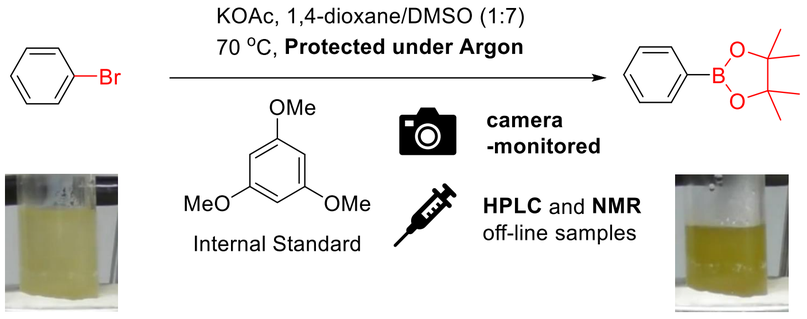
deactivation

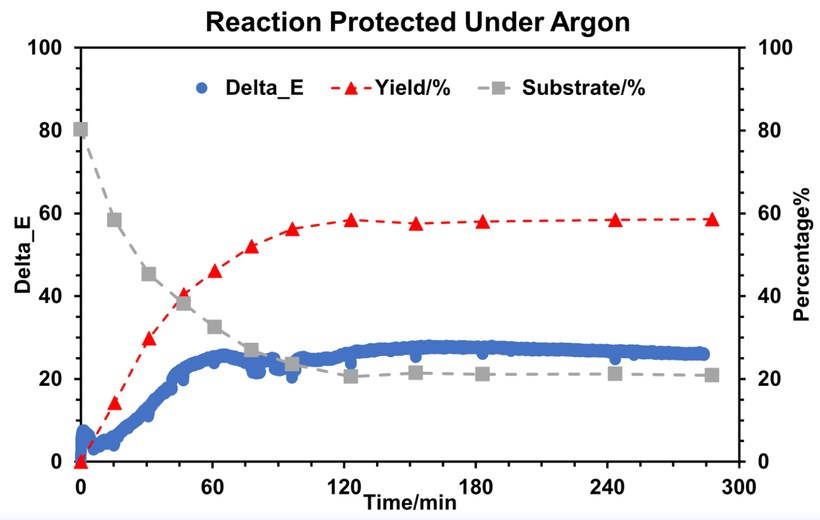
Catalyst Death
'Pd black'
+
$P(O)R_3$

Delta_E – a measurement of *colour* difference.

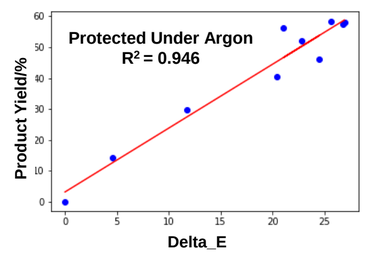


Application in Miyaura Borylation Reaction





Linear Correlation

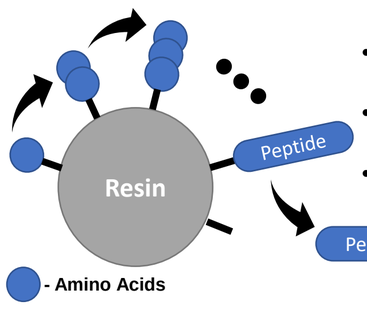


Promising correlations were found between *colour* (from computer vision) and product yield (by NMR).

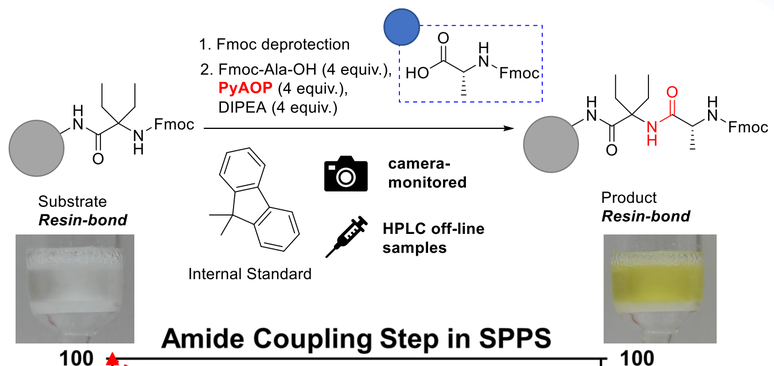
Yet, this linear model breaks when the reaction is exposed to air.

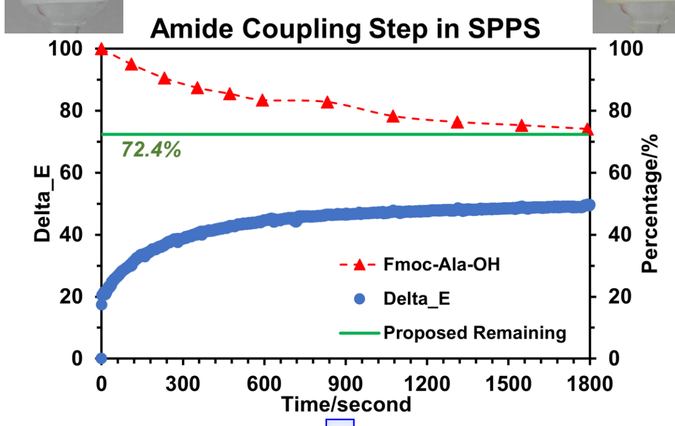
Peptide Synthesis

In Solid Phase



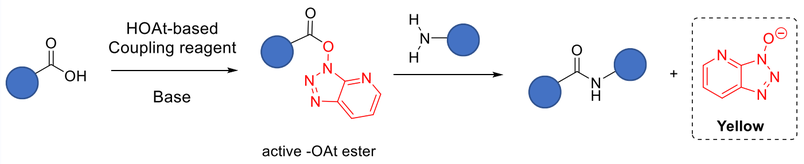
- **Easy Purification** ✓
- **Long Peptides Available** ✓
- **Monitor Reaction Progress** ✗ ***without Intervention***



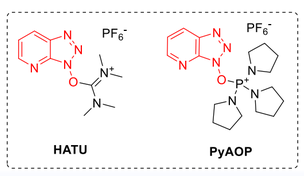


The Coupling Reagent(s)

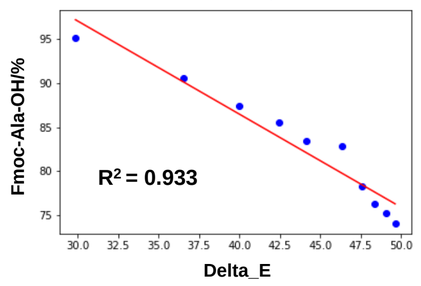
- Forming the amide bond between amino acids requires coupling reagent.[4]

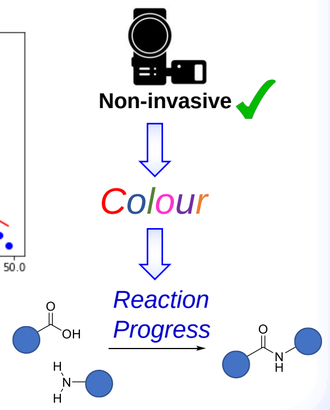


- HOAt based reagents present opportunities to track yellow by-products[5] via computer vision.



Linear Correlation





Summary & Outlook

Pd catalysis

- Quantifiable information on catalyst degradation kinetics is accessible.
- With the linear correlation, simple diagnostic models of reaction success or failure can be build based solely on *colour*.

Peptide Synthesis

- Reaction progress in solid phase can be tracked without any interference based on *colour*
- Possible to realize the self-automation and optimisation of solid-phase peptide synthesis and a wider range of reactions.

Find Out More

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References

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[2] (a) *Meat Sci.*, **2019**, *156*, 183–195.
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[3] *Appl. Catal. A Gen.*, **2001**, *212*, 61–81.
[4] *Tetrahedron*, 2005, **61**, 10827–10852.
[5] *J. Chem. Soc. Chem. Commun.*, 1986, **24**, 1763–1765.

Acknowledgements

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